



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:52 PM UTC

PDB ID : 8J79 / pdb_00008j79
Title : Bovine Xanthine Oxidoreductase Crystallized with oxypurinol
Authors : Okamoto, K.; Sekine, M.
Deposited on : 2023-04-27
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

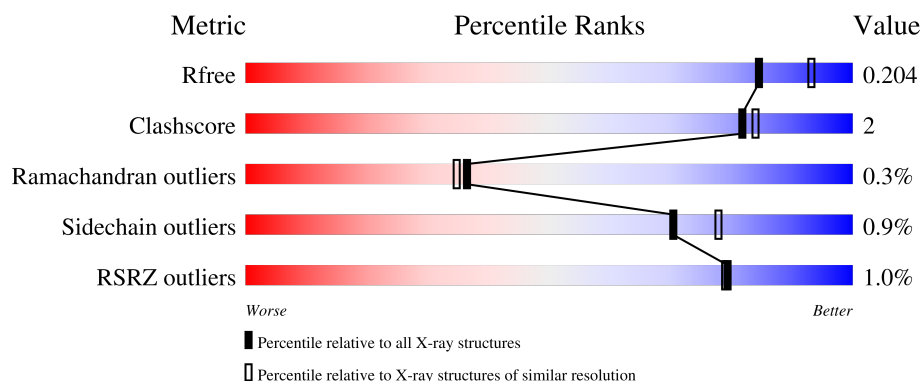
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1332	
1	B	1332	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GOL	B	1413	-	-	X	-

2 Entry composition [i](#)

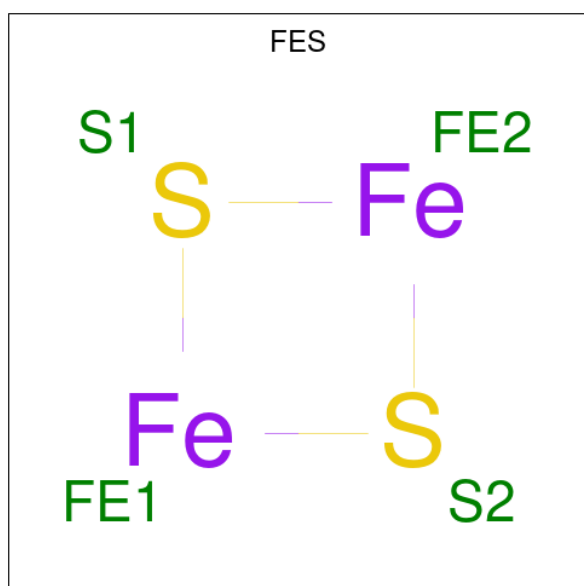
There are 10 unique types of molecules in this entry. The entry contains 22065 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

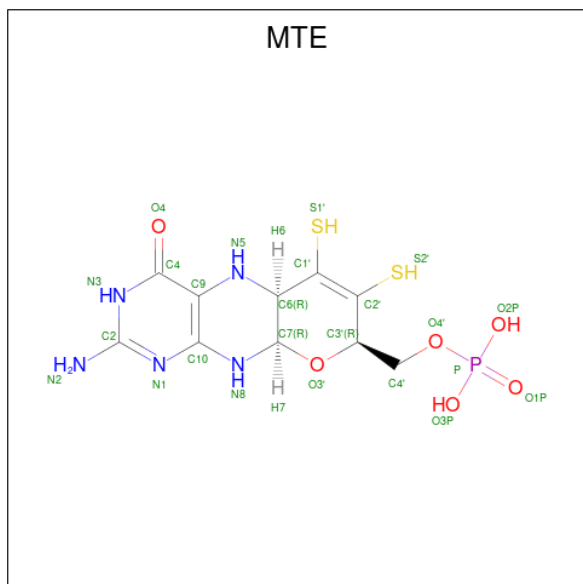
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0	0
			9980	6346	1708	1866	60			
1	B	1288	Total	C	N	O	S	0	0	0
			10000	6358	1711	1870	61			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



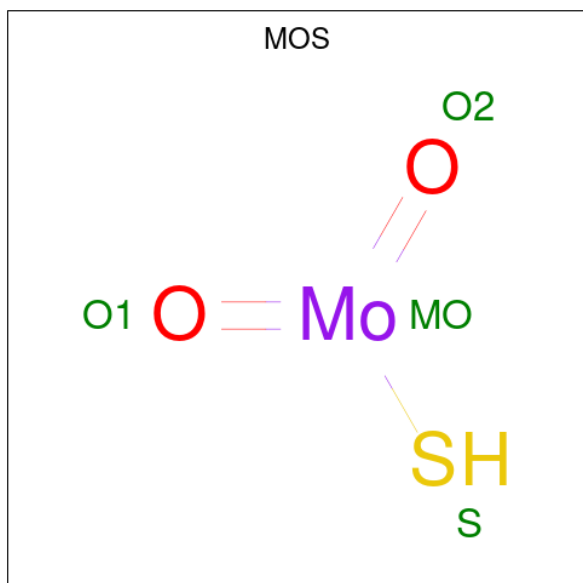
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



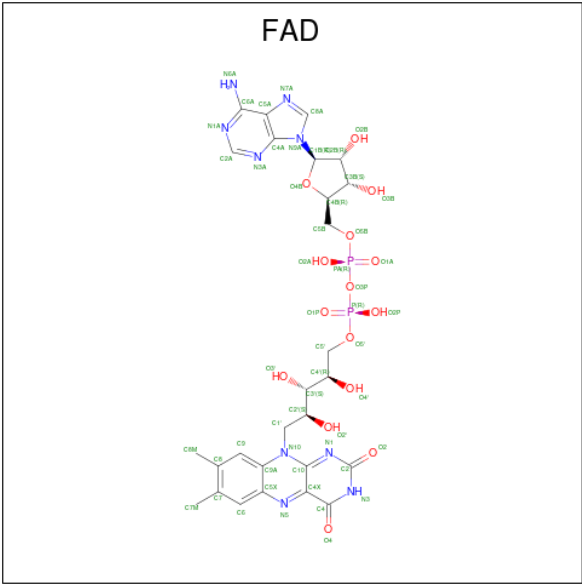
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: $HMoO_2S$).



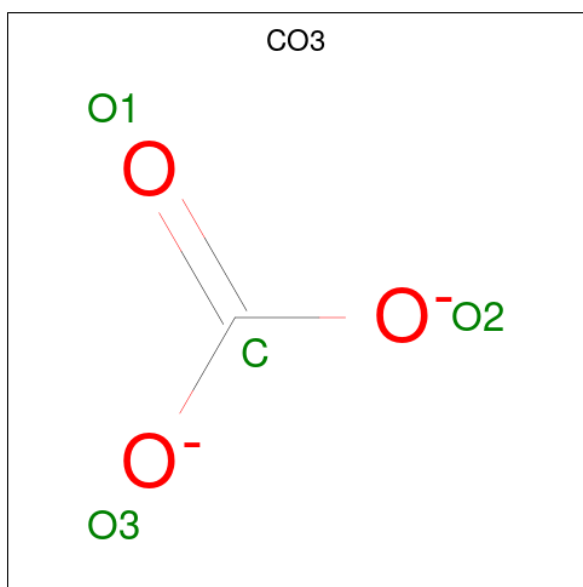
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

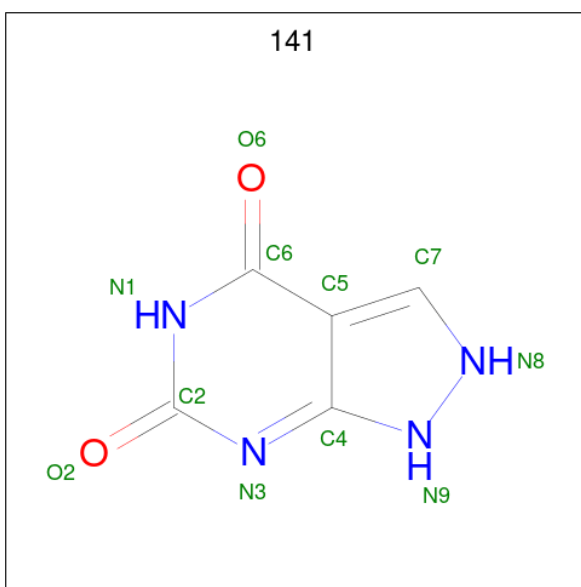


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

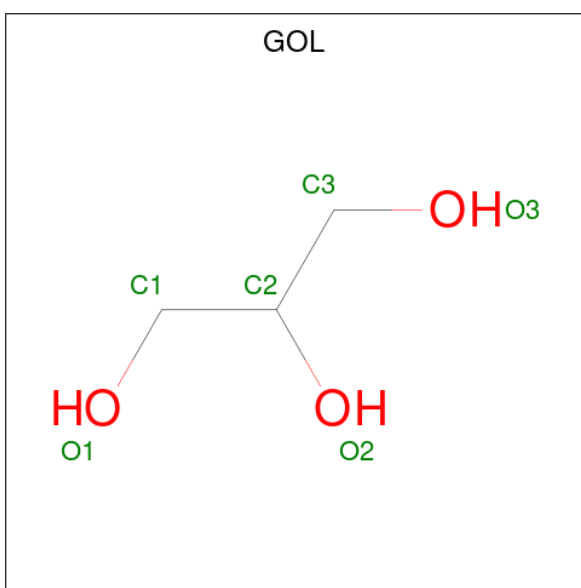
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		

- Molecule 8 is Oxypurinol (CCD ID: 141) (formula: C₅H₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	1
			22	10	8	4		
8	B	1	Total	C	N	O	0	1
			22	10	8	4		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		

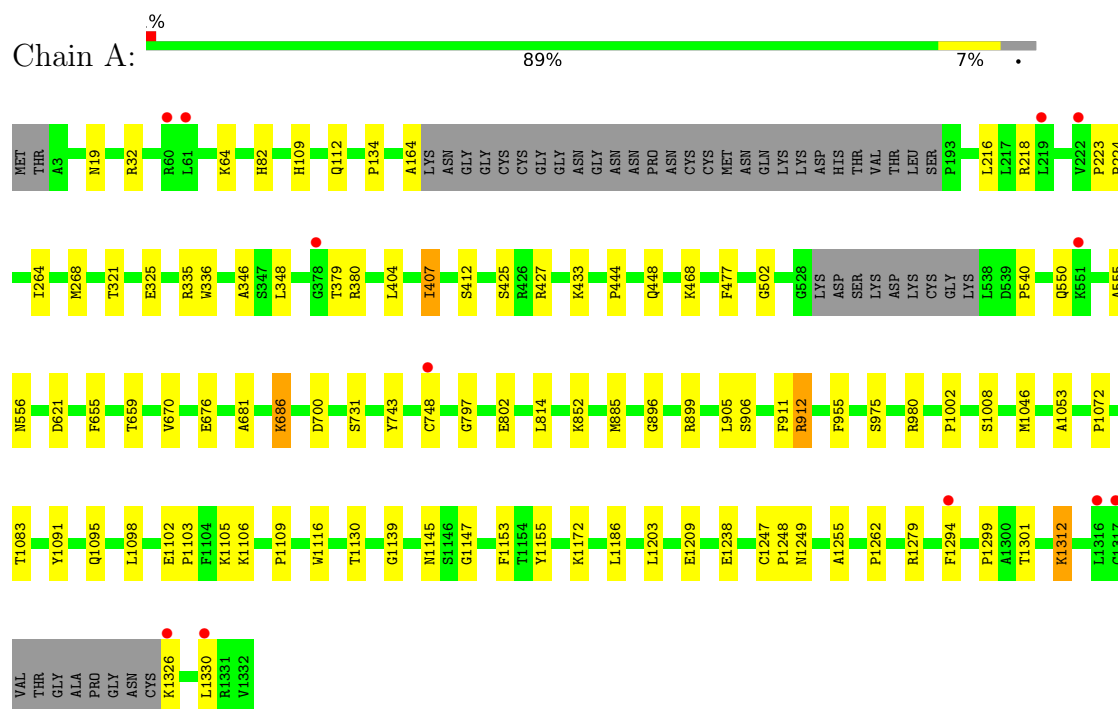
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	928	Total	O	0	0
			928	928		
10	B	887	Total	O	0	0
			887	887		

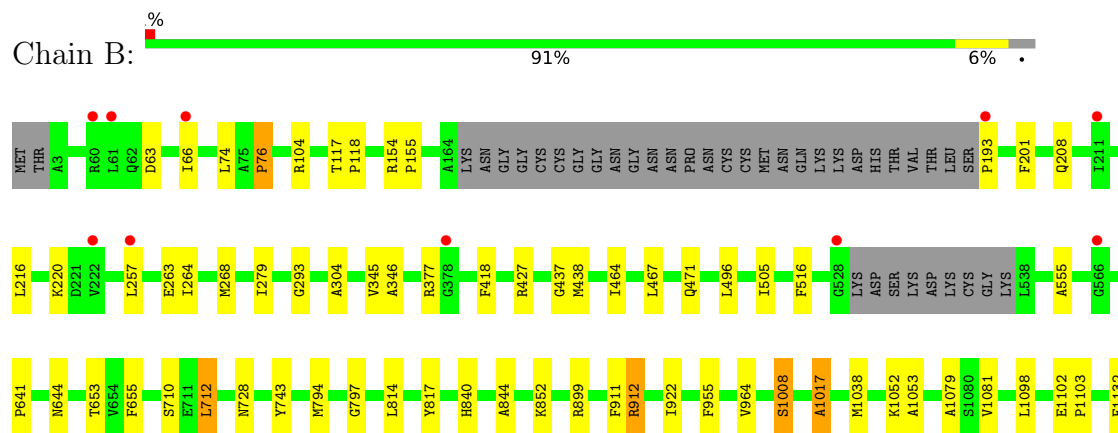
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.68Å 123.47Å 150.06Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	47.72 – 1.99 47.72 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.72-1.99) 99.9 (47.72-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.163 , 0.197 0.171 , 0.204	Depositor DCC
R_{free} test set	10629 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22065	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CA, 141, MTE, CO3, MOS, FAD, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.07	3/10198 (0.0%)	1.28	9/13803 (0.1%)
1	B	1.08	3/10218 (0.0%)	1.29	9/13831 (0.1%)
All	All	1.08	6/20416 (0.0%)	1.28	18/27634 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	840	HIS	CE1-NE2	6.25	1.38	1.32
1	A	444	PRO	C-O	-5.89	1.16	1.24
1	A	540	PRO	C-O	-5.65	1.17	1.24
1	B	76	PRO	C-O	5.36	1.29	1.23
1	B	464	ILE	C-O	5.20	1.29	1.24
1	A	109	HIS	CE1-NE2	5.18	1.37	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1017	ALA	CA-C-N	6.84	126.90	122.18
1	B	1017	ALA	C-N-CA	6.84	126.90	122.18
1	A	700	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	1262	PRO	N-CA-C	6.20	118.26	110.70
1	A	1301	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	1147	GLY	CA-C-O	-5.79	117.60	122.29
1	A	321	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	1130	THR	CA-C-N	5.61	125.93	121.61
1	A	1130	THR	C-N-CA	5.61	125.93	121.61
1	B	1276	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	1262	PRO	N-CA-C	5.49	117.40	110.70
1	B	427	ARG	CB-CA-C	5.47	119.46	110.88
1	B	437	GLY	CA-C-O	-5.47	116.68	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	112	GLN	CA-C-O	-5.22	115.97	119.68
1	A	335	ARG	CB-CA-C	-5.11	102.00	110.68
1	B	964	VAL	N-CA-CB	5.03	113.67	110.50
1	B	1265	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9980	0	9976	48	0
1	B	10000	0	9995	45	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	24	0	10	0	0
3	B	24	0	10	0	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
5	A	53	0	31	4	0
5	B	53	0	31	5	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	22	0	8	2	0
8	B	22	0	8	2	0
9	A	12	0	16	2	0
9	B	24	0	32	6	0
10	A	928	0	0	9	0
10	B	887	0	0	7	0
All	All	22065	0	20117	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1312:LYS:NZ	10:B:1502:HOH:O	2.05	0.80
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.63	0.80
1:A:659:THR:HG21	10:A:1817:HOH:O	1.81	0.79
1:B:63:ASP:O	10:B:1501:HOH:O	2.01	0.77
1:A:19:ASN:ND2	10:A:1501:HOH:O	2.08	0.74
5:B:1405:FAD:C7	9:B:1410:GOL:H32	2.18	0.73
1:B:467:LEU:O	1:B:471:GLN:HG2	1.93	0.69
1:A:380:ARG:NH1	10:A:1506:HOH:O	2.27	0.67
5:A:1405:FAD:C8	9:A:1411:GOL:H32	2.31	0.61
4:A:1404:MOS:O1	8:A:1409[A]:141:O2	2.20	0.59
1:B:345:VAL:HA	9:B:1413:GOL:H11	1.85	0.56
1:A:556:ASN:ND2	10:A:1512:HOH:O	2.37	0.55
1:A:1279:ARG:HG2	1:A:1294:PHE:HE1	1.73	0.54
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.08	0.54
1:B:74:LEU:O	1:B:76:PRO:HD3	2.08	0.53
1:A:346:ALA:HB1	5:A:1405:FAD:H4'	1.90	0.53
1:A:1203:LEU:C	1:A:1203:LEU:HD23	2.34	0.53
1:B:208:GLN:OE1	10:B:1505:HOH:O	2.18	0.53
1:A:425:SER:OG	1:A:433:LYS:NZ	2.42	0.52
1:B:1216:GLU:OE1	10:B:1504:HOH:O	2.17	0.52
4:B:1404:MOS:O1	8:B:1409[A]:141:O2	2.27	0.52
1:A:1312:LYS:NZ	10:A:1502:HOH:O	2.23	0.52
1:A:655:PHE:HE2	1:A:814:LEU:HD23	1.75	0.52
1:B:655:PHE:HE2	1:B:814:LEU:HD23	1.76	0.51
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.10	0.51
1:B:193:PRO:HD2	10:B:1855:HOH:O	2.10	0.51
1:B:257:LEU:O	5:B:1405:FAD:H2B	2.11	0.51
1:A:82:HIS:HA	1:A:216:LEU:HD21	1.93	0.50
1:A:911:PHE:O	1:A:912:ARG:C	2.54	0.50
1:B:712:LEU:HD12	1:B:712:LEU:N	2.27	0.49
1:B:496:LEU:HB2	1:B:505:ILE:HG23	1.94	0.49
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.38	0.49
1:A:1209:GLU:O	1:A:1299:PRO:HG3	2.11	0.48
1:B:346:ALA:HB1	5:B:1405:FAD:H4'	1.97	0.47
1:A:550:GLN:O	1:A:1172:LYS:NZ	2.44	0.47
1:B:304:ALA:HB2	9:B:1413:GOL:H32	1.97	0.47
5:A:1405:FAD:C7	9:A:1411:GOL:H32	2.45	0.47
1:A:134:PRO:O	1:A:164:ALA:HA	2.15	0.47
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.78	0.47
1:A:802:GLU:CD	8:A:1409[A]:141:H4	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:MET:HE2	1:A:1046:MET:HA	1.97	0.46
5:B:1405:FAD:C8	9:B:1410:GOL:H32	2.45	0.46
1:A:218:ARG:NH1	10:A:1527:HOH:O	2.41	0.46
1:B:293:GLY:O	10:B:1506:HOH:O	2.20	0.46
1:A:502:GLY:HA3	10:A:2203:HOH:O	2.15	0.46
1:B:641:PRO:HG3	1:B:817:TYR:CE2	2.50	0.46
1:B:852:LYS:HD3	10:B:1688:HOH:O	2.15	0.46
1:B:955:PHE:HA	1:B:1145:ASN:OD1	2.16	0.46
1:B:257:LEU:HA	1:B:279:ILE:O	2.15	0.45
1:B:1079:ALA:HB2	8:B:1409[B]:141:C7	2.46	0.45
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.99	0.45
1:A:655:PHE:CE2	1:A:814:LEU:HD23	2.52	0.45
1:A:1105:LYS:HE2	1:A:1116:TRP:CZ3	2.51	0.45
1:B:104:ARG:HD3	1:B:201:PHE:CD2	2.52	0.45
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.25	0.44
1:A:1106:LYS:O	1:A:1109:PRO:HD3	2.17	0.44
1:A:325:GLU:HB2	1:A:412:SER:HB3	2.00	0.44
1:B:345:VAL:HA	9:B:1413:GOL:C1	2.48	0.44
1:B:154:ARG:N	1:B:155:PRO:HD2	2.34	0.43
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	2.00	0.43
1:A:555:ALA:O	1:A:1238:GLU:HA	2.18	0.43
1:A:1083:THR:HG21	1:A:1186:LEU:HD12	2.01	0.43
1:A:885:MET:SD	1:A:896:GLY:HA3	2.59	0.43
1:B:117:THR:HB	1:B:118:PRO:HD3	2.00	0.43
1:A:975:SER:O	1:A:980:ARG:HD3	2.18	0.43
1:A:1247:CYS:N	1:A:1248:PRO:CD	2.81	0.43
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.90	0.43
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.43	0.42
1:A:268:MET:HE1	10:A:2133:HOH:O	2.19	0.42
1:B:794:MET:HE3	1:B:1038:MET:HB3	2.02	0.42
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.01	0.42
1:A:336:TRP:CZ3	1:A:427:ARG:HG2	2.55	0.42
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.55	0.42
1:A:264:ILE:HD11	5:A:1405:FAD:H3B	2.02	0.42
1:A:1326:LYS:NZ	10:A:1572:HOH:O	2.53	0.42
1:B:345:VAL:HA	9:B:1413:GOL:H2	2.01	0.42
1:B:644:ASN:O	1:B:653:THR:HA	2.20	0.42
1:B:1052:LYS:HD3	1:B:1254:TYR:CZ	2.55	0.42
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.20	0.41
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.95	0.41
1:B:728:ASN:OD1	1:B:852:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:ARG:HA	1:B:899:ARG:HD2	1.90	0.41
1:B:911:PHE:O	1:B:912:ARG:C	2.64	0.41
1:B:418:PHE:HA	1:B:438:MET:O	2.21	0.41
1:B:1017:ALA:O	1:B:1132:PHE:HA	2.21	0.41
1:A:621:ASP:HB3	1:A:686:LYS:HE3	2.02	0.41
1:A:955:PHE:HA	1:A:1145:ASN:OD1	2.21	0.41
1:B:63:ASP:O	1:B:63:ASP:CG	2.63	0.41
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.21	0.40
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.21	0.40
1:A:448:GLN:HB2	1:A:477:PHE:CE2	2.56	0.40
1:B:555:ALA:O	1:B:1238:GLU:HA	2.21	0.40
1:A:468:LYS:HE2	1:A:468:LYS:HB3	1.95	0.40
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.40
1:A:905:LEU:O	1:A:906:SER:C	2.65	0.40
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	2.04	0.40
1:B:263:GLU:HB2	5:B:1405:FAD:H52A	2.02	0.40
1:B:264:ILE:O	1:B:268:MET:HG3	2.21	0.40
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1277/1332 (96%)	1235 (97%)	38 (3%)	4 (0%)	36	35
1	B	1280/1332 (96%)	1248 (98%)	28 (2%)	4 (0%)	36	35
All	All	2557/2664 (96%)	2483 (97%)	66 (3%)	8 (0%)	36	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	912	ARG
1	A	1008	SER
1	B	1008	SER
1	B	912	ARG
1	A	797	GLY
1	B	1139	GLY
1	A	1139	GLY
1	B	797	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1090/1128 (97%)	1077 (99%)	13 (1%)	63	70
1	B	1093/1128 (97%)	1086 (99%)	7 (1%)	78	85
All	All	2183/2256 (97%)	2163 (99%)	20 (1%)	70	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	379	THR
1	A	407	ILE
1	A	686	LYS
1	A	731	SER
1	A	743	TYR
1	A	748	CYS
1	A	852	LYS
1	A	899	ARG
1	A	1002	PRO
1	A	1072	PRO
1	A	1312	LYS
1	A	1330	LEU
1	B	66	ILE
1	B	220	LYS
1	B	377	ARG

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Mol	Chain	Res	Type
1	B	710	SER
1	B	712	LEU
1	B	743	TYR
1	B	1288	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	484	GLN
1	A	875	HIS
1	A	1220	HIS
1	B	71	ASN
1	B	322	GLN
1	B	333	GLN
1	B	1122	GLN
1	B	1288	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MOS	A	1404	3	0,3,3	-	-	-		
2	FES	A	1402	1	0,4,4	-	-	-		
9	GOL	A	1410	-	5,5,5	0.11	0	5,5,5	0.31	0
9	GOL	A	1411	-	5,5,5	0.19	0	5,5,5	0.59	0
4	MOS	B	1404	3	0,3,3	-	-	-		
9	GOL	B	1412	-	5,5,5	0.19	0	5,5,5	0.31	0
2	FES	B	1401	1	0,4,4	-	-	-		
8	141	B	1409[A]	-	11,12,12	1.84	2 (18%)	11,17,17	0.87	0
8	141	A	1409[B]	-	11,12,12	1.69	2 (18%)	11,17,17	1.03	0
6	CO3	A	1406	-	3,3,3	0.59	0	2,3,3	0.35	0
2	FES	B	1402	1	0,4,4	-	-	-		
5	FAD	B	1405	-	58,58,58	0.67	0	85,89,89	0.74	1 (1%)
9	GOL	B	1411	-	5,5,5	0.11	0	5,5,5	0.37	0
2	FES	A	1401	1	0,4,4	-	-	-		
8	141	B	1409[B]	-	11,12,12	1.72	2 (18%)	11,17,17	0.91	0
9	GOL	B	1413	-	5,5,5	0.27	0	5,5,5	0.65	0
3	MTE	B	1403	4	21,26,26	0.92	0	19,40,40	2.00	6 (31%)
5	FAD	A	1405	-	58,58,58	0.72	1 (1%)	85,89,89	0.73	1 (1%)
3	MTE	A	1403	4	21,26,26	1.08	1 (4%)	19,40,40	2.00	5 (26%)
9	GOL	B	1410	-	5,5,5	0.15	0	5,5,5	0.61	0
8	141	A	1409[A]	-	11,12,12	2.22	2 (18%)	11,17,17	0.77	0
6	CO3	B	1406	-	3,3,3	0.73	0	2,3,3	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	1402	1	-	-	0/1/1/1
3	MTE	B	1403	4	-	3/6/34/34	0/3/3/3
2	FES	B	1402	1	-	-	0/1/1/1
3	MTE	A	1403	4	-	3/6/34/34	0/3/3/3
5	FAD	B	1405	-	-	2/34/50/50	0/6/6/6
5	FAD	A	1405	-	-	2/34/50/50	0/6/6/6
9	GOL	A	1410	-	-	2/4/4/4	-
9	GOL	A	1411	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	B	1410	-	-	0/4/4/4	-
9	GOL	B	1411	-	-	4/4/4/4	-
9	GOL	B	1412	-	-	0/4/4/4	-
8	141	A	1409[A]	-	-	-	0/2/2/2
2	FES	B	1401	1	-	-	0/1/1/1
8	141	B	1409[A]	-	-	-	0/2/2/2
2	FES	A	1401	1	-	-	0/1/1/1
8	141	A	1409[B]	-	-	-	0/2/2/2
8	141	B	1409[B]	-	-	-	0/2/2/2
9	GOL	B	1413	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1409[A]	141	C7-N8	6.14	1.38	1.33
8	B	1409[A]	141	C7-N8	4.66	1.37	1.33
8	B	1409[B]	141	C7-N8	4.18	1.36	1.33
8	A	1409[B]	141	C5-C4	-3.32	1.39	1.45
8	B	1409[A]	141	C5-C4	-3.11	1.40	1.45
8	A	1409[B]	141	C7-N8	3.01	1.35	1.33
8	A	1409[A]	141	C5-C4	-2.91	1.40	1.45
5	A	1405	FAD	PA-O3P	2.78	1.62	1.59
8	B	1409[B]	141	C5-C4	-2.61	1.41	1.45
3	A	1403	MTE	C7-C6	-2.05	1.52	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1403	MTE	O3'-C7-N8	5.67	113.75	108.61
3	B	1403	MTE	O3'-C7-N8	3.52	111.80	108.61
3	B	1403	MTE	C2-N1-C10	3.39	119.34	113.36
3	B	1403	MTE	O3P-P-O4'	-3.10	98.58	106.67
3	B	1403	MTE	O4'-P-O1P	-2.75	99.02	106.44
3	A	1403	MTE	C7-C6-N5	2.63	110.45	107.87
3	A	1403	MTE	C2-N1-C10	2.62	117.98	113.36
3	B	1403	MTE	O4'-C4'-C3'	2.39	114.47	108.58
3	A	1403	MTE	O3P-P-O4'	-2.30	100.67	106.67
5	A	1405	FAD	O2A-PA-O1A	2.30	123.14	112.44
5	B	1405	FAD	O2A-PA-O1A	2.15	122.43	112.44
3	B	1403	MTE	C7-C6-N5	2.10	109.93	107.87
3	A	1403	MTE	O3'-C7-C6	-2.02	107.62	108.96

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1403	MTE	C4'-O4'-P-O3P
3	B	1403	MTE	C4'-O4'-P-O1P
5	A	1405	FAD	N10-C1'-C2'-O2'
5	A	1405	FAD	N10-C1'-C2'-C3'
5	B	1405	FAD	N10-C1'-C2'-O2'
5	B	1405	FAD	N10-C1'-C2'-C3'
9	A	1410	GOL	O1-C1-C2-O2
9	A	1410	GOL	O1-C1-C2-C3
9	B	1411	GOL	O1-C1-C2-C3
9	B	1413	GOL	C1-C2-C3-O3
9	A	1411	GOL	C1-C2-C3-O3
9	B	1411	GOL	C1-C2-C3-O3
9	B	1413	GOL	O1-C1-C2-C3
9	A	1411	GOL	O2-C2-C3-O3
9	B	1413	GOL	O2-C2-C3-O3
9	B	1411	GOL	O2-C2-C3-O3
3	B	1403	MTE	C3'-C4'-O4'-P
9	B	1411	GOL	O1-C1-C2-O2
3	B	1403	MTE	C4'-O4'-P-O3P
3	A	1403	MTE	C3'-C4'-O4'-P
3	A	1403	MTE	C4'-O4'-P-O2P

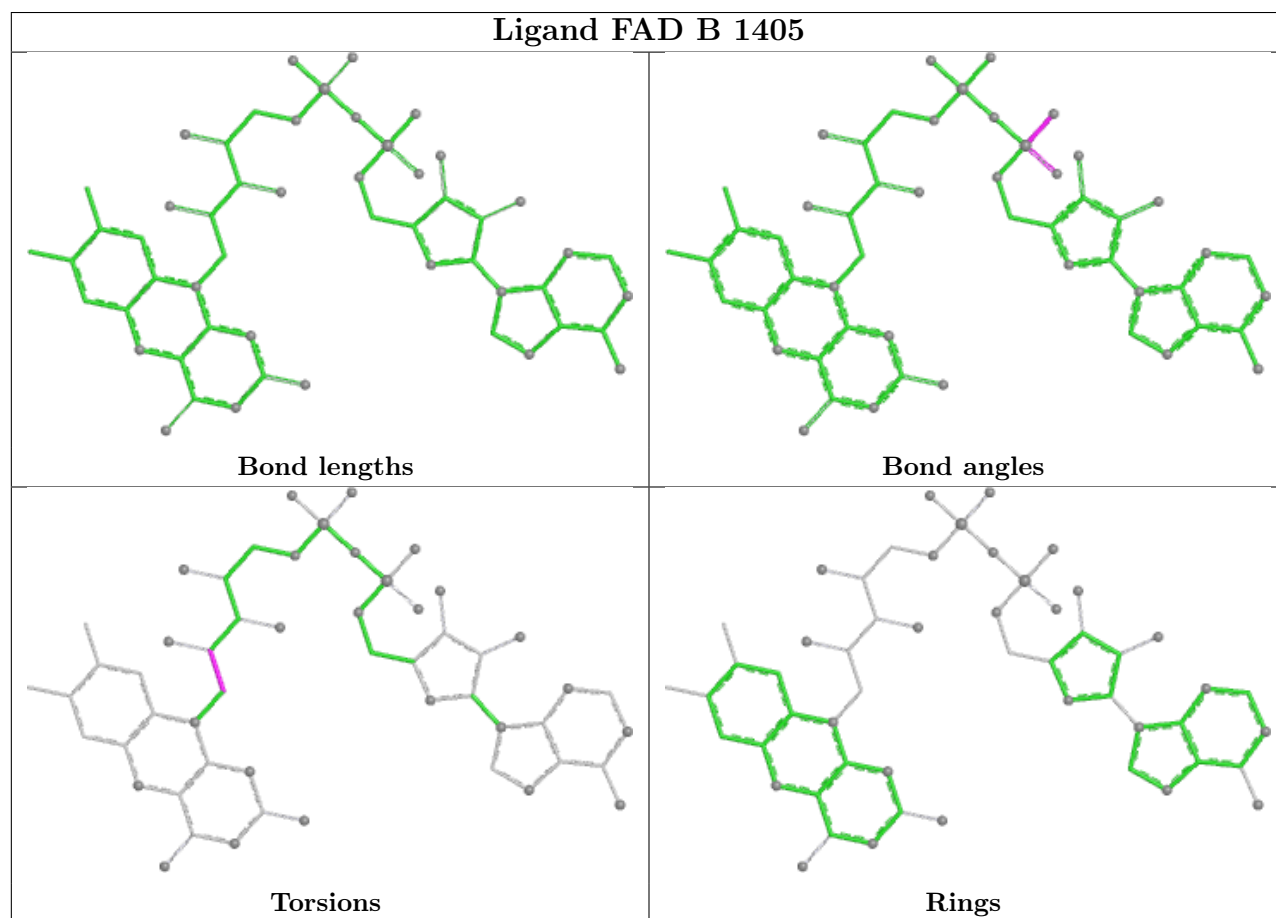
There are no ring outliers.

10 monomers are involved in 17 short contacts:

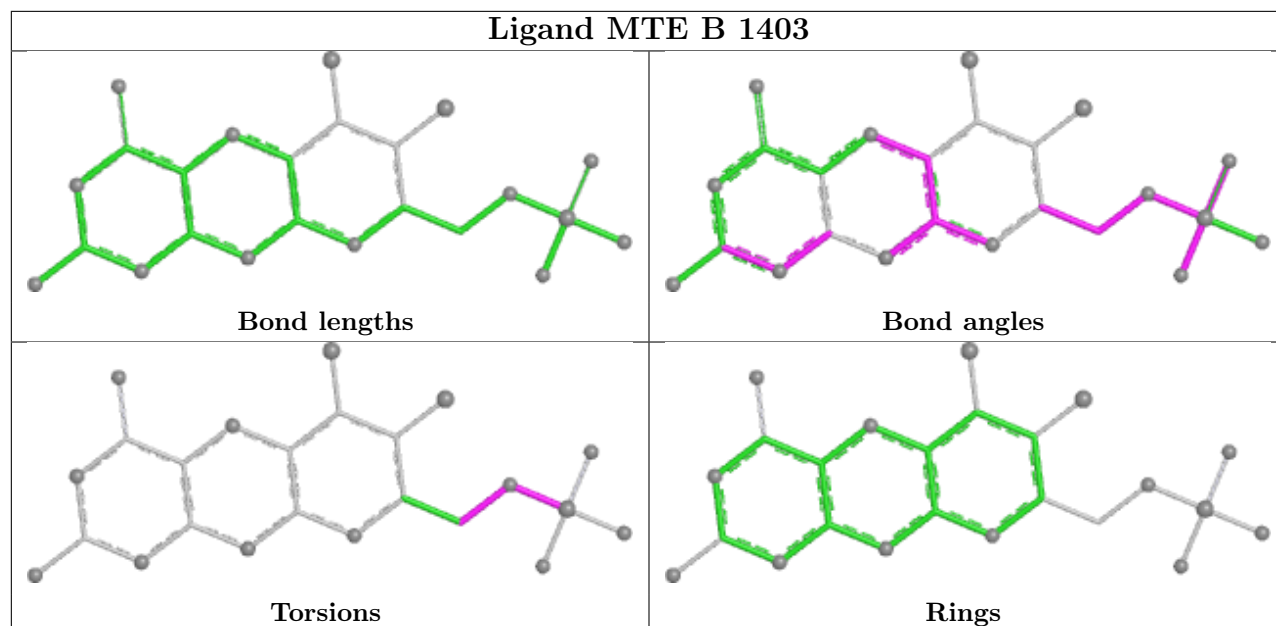
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1404	MOS	1	0
9	A	1411	GOL	2	0
4	B	1404	MOS	1	0
8	B	1409[A]	141	1	0
5	B	1405	FAD	5	0
8	B	1409[B]	141	1	0
9	B	1413	GOL	4	0
5	A	1405	FAD	4	0
9	B	1410	GOL	2	0
8	A	1409[A]	141	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

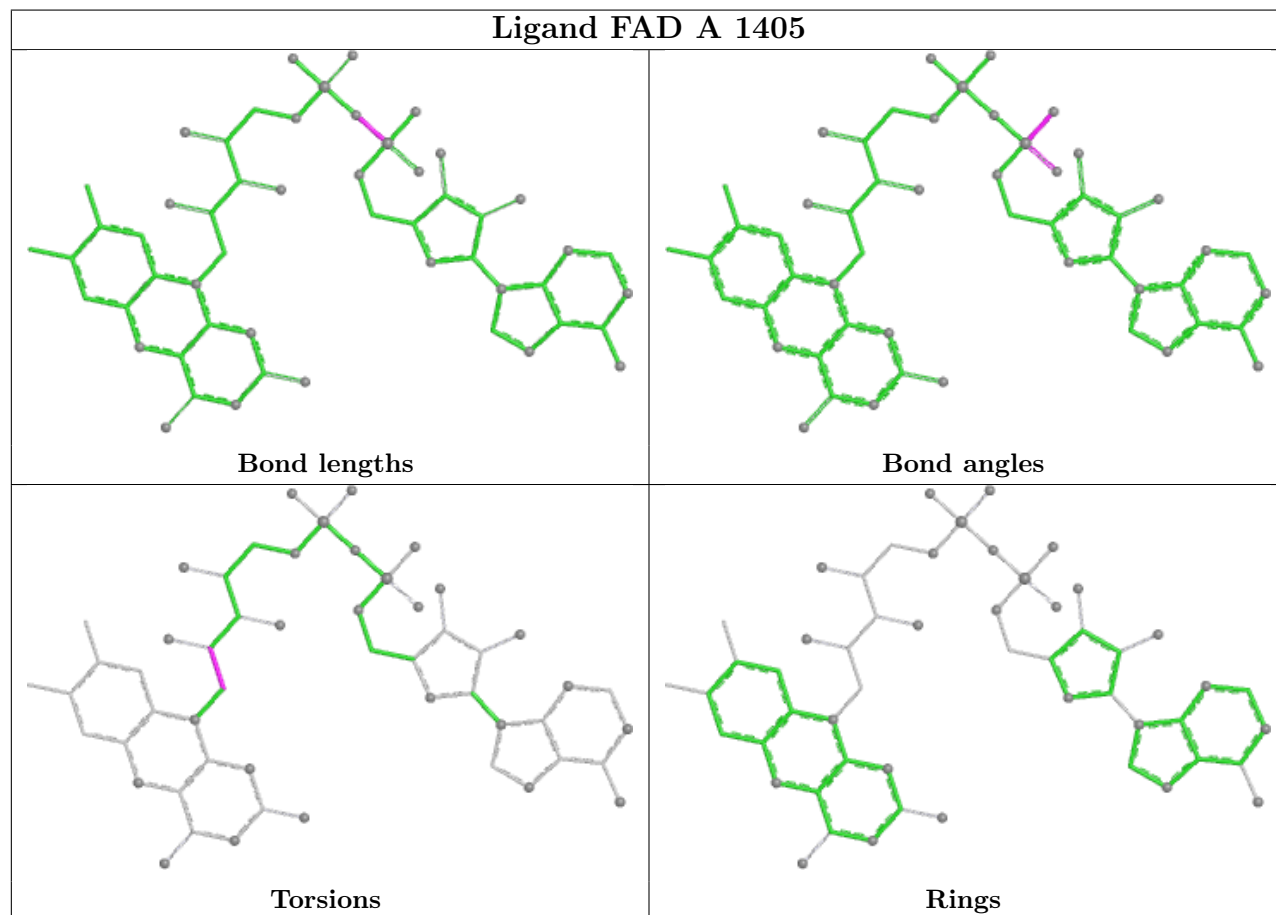
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

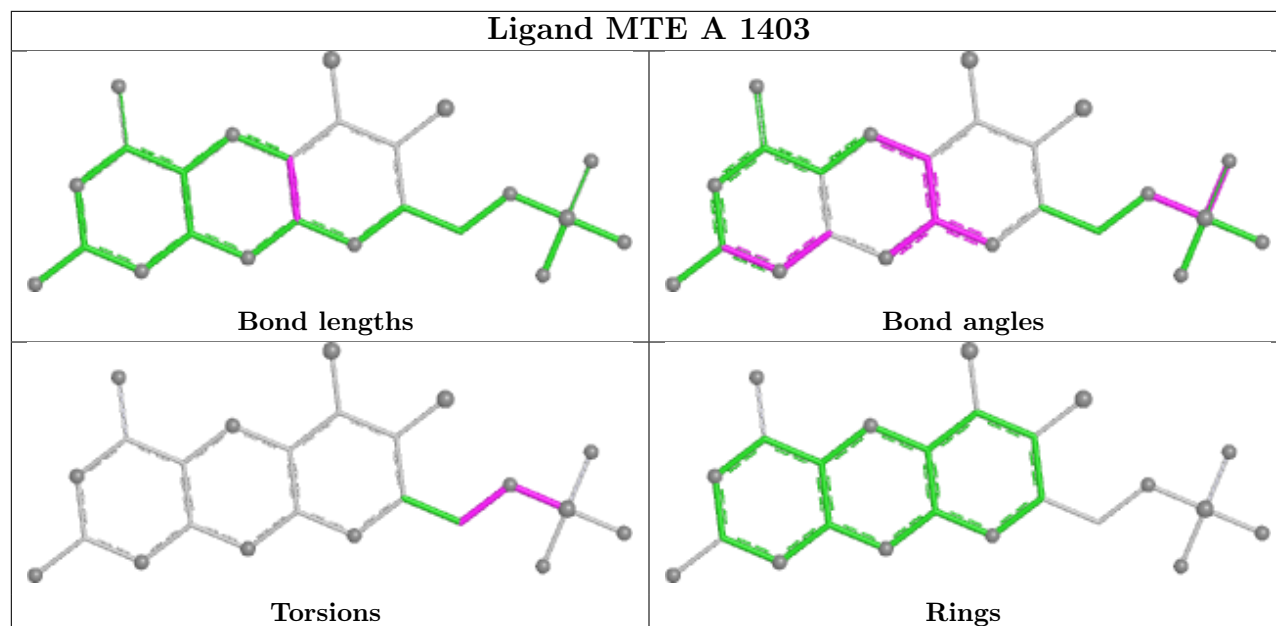


Ligand MTE B 1403



Ligand FAD A 1405





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1285/1332 (96%)	-0.07	12 (0%) 81 80	19, 29, 46, 80	0
1	B	1288/1332 (96%)	-0.06	13 (1%) 79 79	19, 29, 47, 78	0
All	All	2573/2664 (96%)	-0.07	25 (0%) 79 79	19, 29, 47, 80	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	LEU	4.7
1	A	61	LEU	3.5
1	A	222	VAL	3.2
1	B	566	GLY	3.1
1	A	1317	CYS	3.1
1	B	193	PRO	3.0
1	A	60	ARG	2.9
1	A	551	LYS	2.9
1	B	1325	CYS	2.8
1	A	1326	LYS	2.7
1	A	1316	LEU	2.6
1	B	378	GLY	2.5
1	B	1288	ASN	2.4
1	B	211	ILE	2.4
1	B	1319	THR	2.3
1	A	378	GLY	2.3
1	A	748	CYS	2.3
1	B	528	GLY	2.3
1	A	1330	LEU	2.3
1	B	66	ILE	2.2
1	B	60	ARG	2.2
1	A	219	LEU	2.1
1	B	257	LEU	2.1
1	A	1294	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

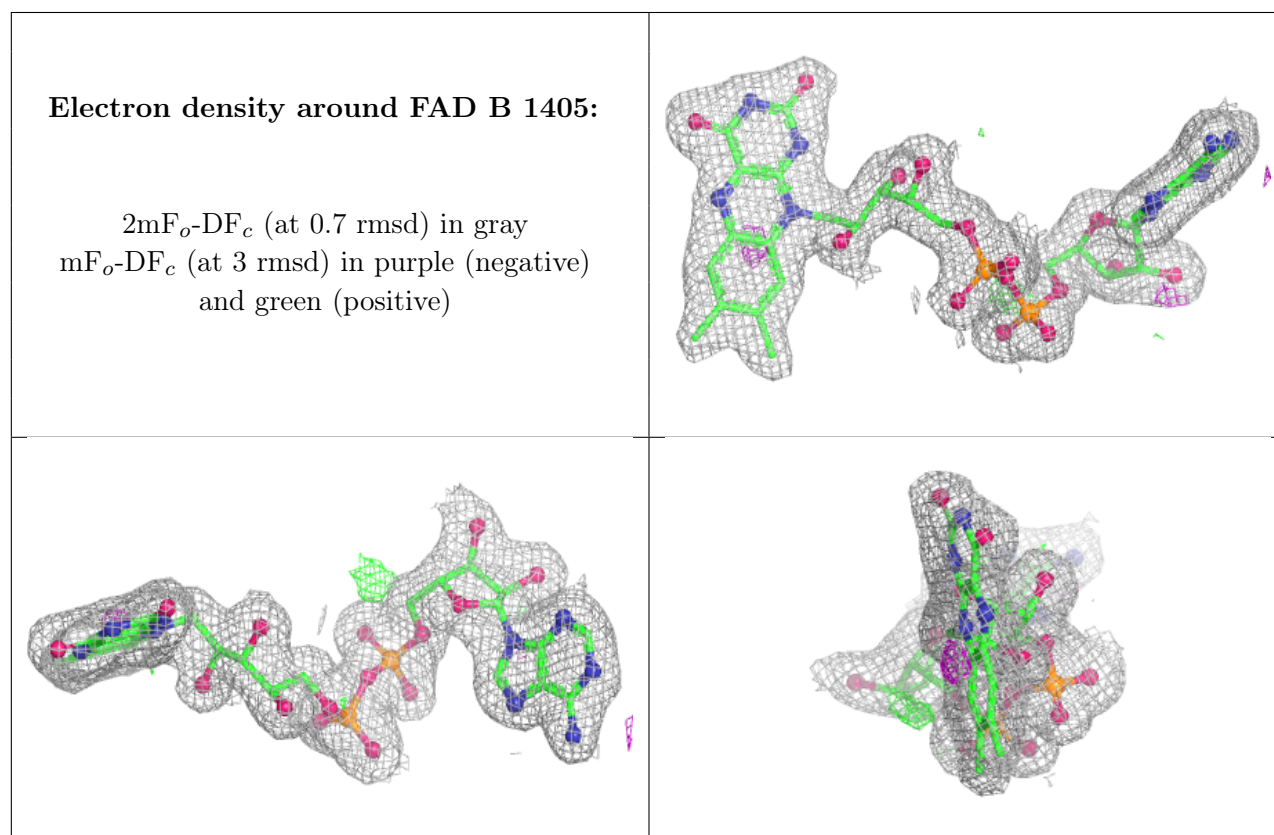
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	141	B	1409[A]	11/11	0.75	0.18	35,42,45,53	11
8	141	B	1409[B]	11/11	0.75	0.18	30,40,43,44	11
8	141	A	1409[A]	11/11	0.79	0.14	26,31,34,35	11
8	141	A	1409[B]	11/11	0.79	0.14	30,36,40,40	11
9	GOL	B	1412	6/6	0.83	0.16	42,54,58,58	0
9	GOL	B	1411	6/6	0.84	0.18	47,57,60,64	0
9	GOL	B	1413	6/6	0.85	0.18	25,27,28,30	6
9	GOL	B	1410	6/6	0.86	0.15	52,53,55,55	0
9	GOL	A	1411	6/6	0.87	0.14	50,51,52,55	0
9	GOL	A	1410	6/6	0.90	0.14	37,50,53,56	0
6	CO3	A	1406	4/4	0.97	0.06	21,23,24,24	0
6	CO3	B	1406	4/4	0.97	0.05	23,27,27,28	0
5	FAD	B	1405	53/53	0.97	0.06	22,25,30,32	0
3	MTE	B	1403	24/24	0.98	0.05	16,23,26,28	0
5	FAD	A	1405	53/53	0.98	0.05	22,27,32,33	0
3	MTE	A	1403	24/24	0.98	0.04	16,23,29,32	0
7	CA	B	1407	1/1	0.99	0.04	25,25,25,25	0
7	CA	B	1408	1/1	0.99	0.06	29,29,29,29	0
4	MOS	B	1404	4/4	0.99	0.06	27,27,34,40	0
7	CA	A	1408	1/1	0.99	0.08	29,29,29,29	0
2	FES	B	1402	4/4	1.00	0.02	21,22,22,23	0
2	FES	A	1401	4/4	1.00	0.02	20,21,22,22	0

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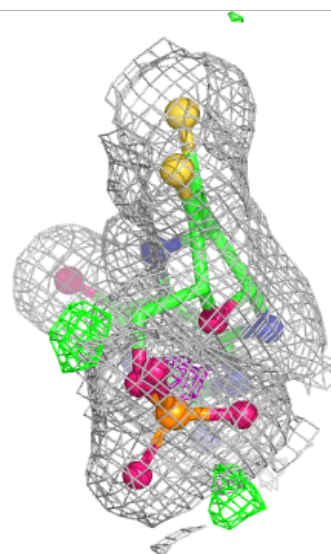
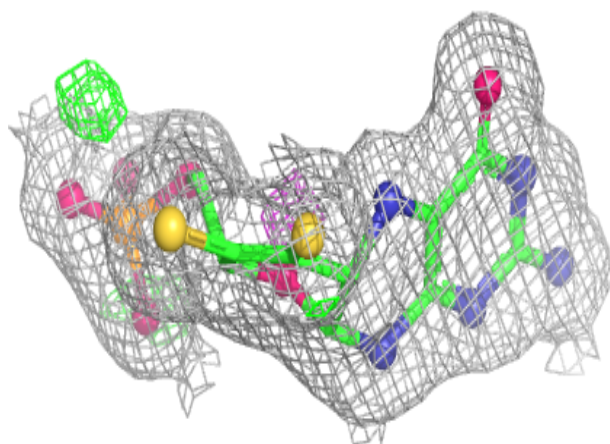
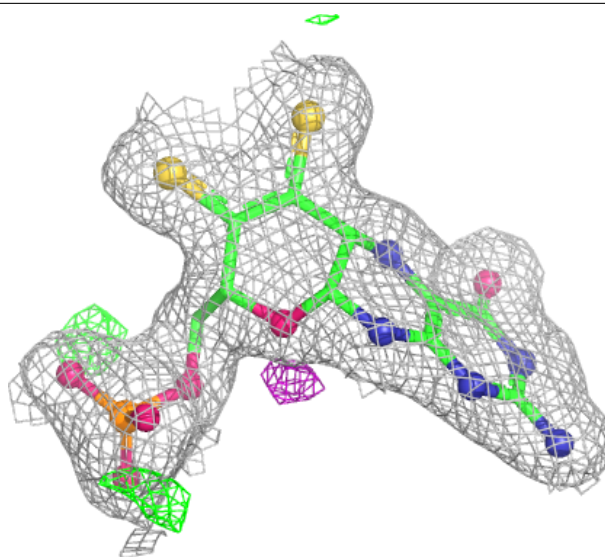
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FES	A	1402	4/4	1.00	0.02	23,23,24,25	0
4	MOS	A	1404	4/4	1.00	0.06	28,31,32,41	0
7	CA	A	1407	1/1	1.00	0.02	24,24,24,24	0
2	FES	B	1401	4/4	1.00	0.02	21,21,21,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



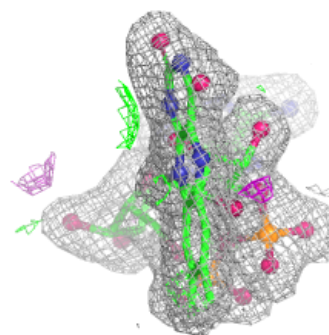
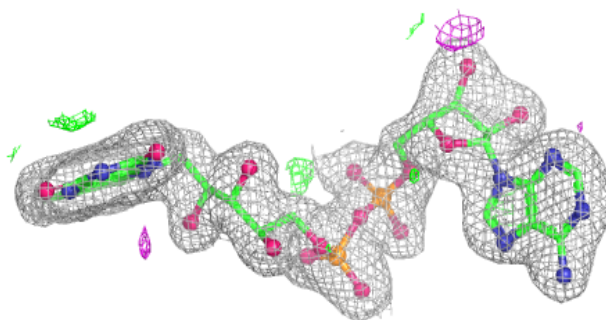
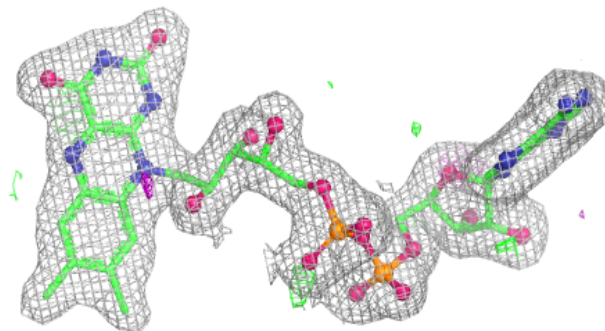
Electron density around MTE B 1403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



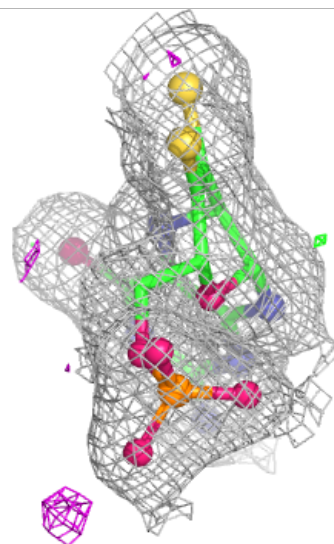
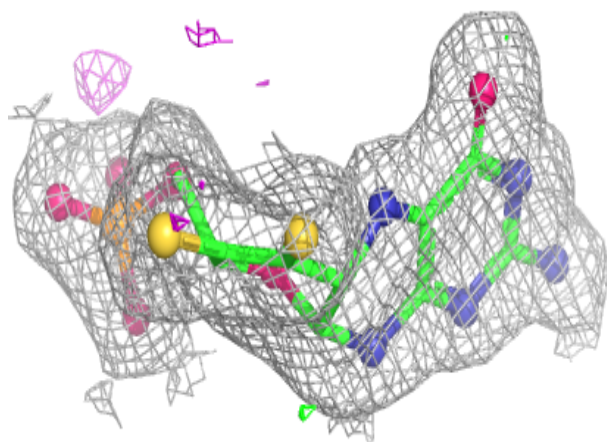
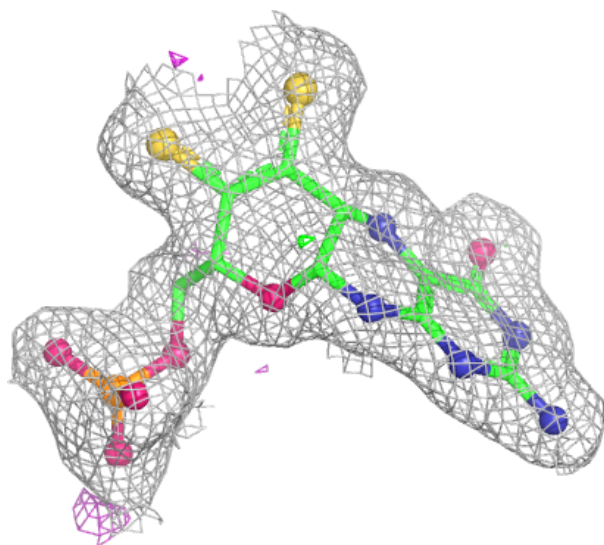
Electron density around FAD A 1405:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTE A 1403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.